Added value of the emissions fractions approach when assessing a chemical's potential for adverse effects as a result of long-range transport

SUPPORTING INFORMATION

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Table of Contents

S1. Transfer Efficiency

Wegmann et al. recognized that TE may exceed 100% for chemicals which undergo reversible atmospheric deposition.[1] From Figure 2d we also see that the predicted net transfer efficiency (TE_{net}) for some chemicals still exceeds 100%. This is because the dispersion of chemicals via advective outflow in air from the source region is additionally dependent on the selected cross-sectional area ($Aadv_A$) which connects the source and remote regions.[2] In the case of TE and TE_{net}, $Aadv_A$ relies on the default approach in The Tool for which $Aadv_A$ equals the square root of the global surface area times the height of the air compartment.[1] When calculating the alternative metrics (EFA) the calculated cross-sectional area was fitted in order for $\phi 1_A$ ($\phi 1$ for dispersion via air only) to adopt a maximum value of 1.[2] If the default cross-sectional areas were harmonized to align with the EFA, then TE_{net} and $\phi 2_A$ (net atmospheric deposition in the remote region as a consequence of dispersion via air only) would be the same.

Table S1. Chemical name, CAS number, molecular weight, physical-chemical properties (25°C) and environmental degradation half-lives (25°C) for selected chemicals.[3]

IUPAC Name	CAS	MW (g/mol)	log K_{AW} (-)	log K_{OW} (-)	$t_{1/2}$ air (h)	$t_{1/2}$ water (h)	$t_{1/2}$ soil (h)	Figures
1,2,3,4-tetrachlorobenzene	634-66-2	215.9	-1.47	4.60	2,341	3,937	7,874	4 / S2a
3,9-dibromo-7H-benzo[de]anthracen-7-one	81-98-1	388.1	-6.33	6.51	27.6	2,499	4,999	4 / S2b
2,2'-di(propan-2-yl)biphenyl	36876-13-8	238.4	-1.16	6.67	15.2	4,078	8,155	4 / S2c
Docosanamide	3061-75-4	339.6	-3.84	8.66	5.9	239	477	5 / S3a
Bromoform	75-25-2	252.7	-1.62	2.40	4,521	761	1,522	5 / S3b
1-chloro-2-[chloro(diphenyl)methyl]benzene	42074-68-0	313.2	-3.35	6.23	18.8	2,823	5,645	5 / S3c
1,1,1,3,3,3-hexafluoropropan-2-ol	920-66-1	168.0	-2.72	1.66	7,463	2,290	4,580	5 / S3d
1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro-1,4:5,8-dimethanonaphthalene	309-00-2	364.9	-1.76	6.06	1	25,760	51,520	5 / S3e
1,2,3,4,7,8-hexabromocyclodecane	3194-55-6	613.7	-4.36	6.76	53.9	3,931	7,862	5 / S3f

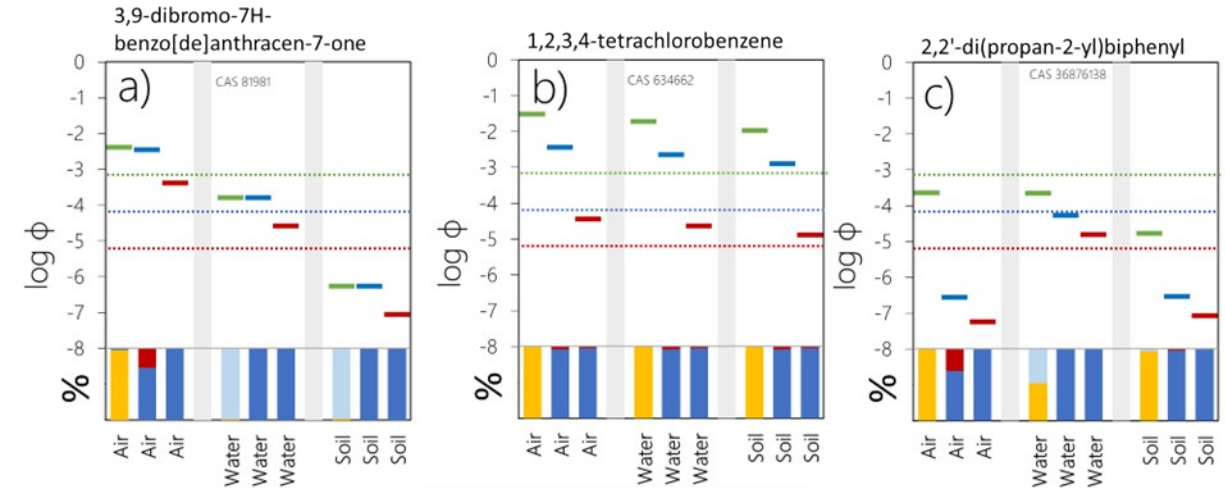
Table S2. Predicted CTD, TE, P_{OV}, log ϕ1, log ϕ2, and log ϕ3 using the existing and EFA metrics for selected chemicals.

IUPAC Name	CTD_{air} (km)	CTD_{water} (km)	TE (%)	P_{OV} (days)	log ϕ1	log ϕ2	log ϕ3
1,2,3,4-tetrachlorobenzene	**41,519**	182	**55.2**	361	-1.51	-2.45	-4.43
3,9-dibromo-7H-benzo[de]anthracen-7-one	**5,543**	218	**20.5**	300	-2.38	-2.45	-3.38
2,2'-di(propan-2-yl)biphenyl	315	147	0.002	455	-3.63	-4.27	-4.79
Docosanamide	2,250	22	**3.320**	29	-2.78	-3.25	-4.30
Bromoform	**52,900**	68	**124**	178	-1.41	-1.81	-4.69
1-chloro-2-[chloro(diphenyl)methyl]benzene	383	202	0.112	338	-3.53	-3.92	-4.89
1,1,1,3,3,3-hexafluoropropan-2-ol	**17,020**	226	**109**	174	-1.89	-1.95	-4.37
1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro-1,4:5,8-dimethanonaphthalene	20	226	<0.000	**2,059**	-3.75	-4.60	-4.96
1,2,3,4,7,8-hexabromocyclodecane	**1,642**	268	**2.28**	472	-2.90	-3.37	-3.91

Table S3. CAS, molecular weight, physical-chemical properties (25°C), environmental degradation half-lives (25°C) for methoxychlor[4], UV-328[5] and chlorpyrifos[6], including predicted metrics.

Chemical name	CAS	MW (g/mol)	log K_{AW} (-)	log K_{OW} (-)	$t_{1/2}$ air (h)	$t_{1/2}$ water (h)	$t_{1/2}$ soil (h)	CTD (km)	TE (%)	P_{OV} (days)	log $\phi 1$	log $\phi 2$	log $\phi 3$
Methoxychlor	72-43-5	345.7	-5.08	5.08	5	4,992	5,040	498	0.01	303	-3.43	-3.44	-5.07
UV-328	25973-55-1	351.5	-2.76	8.53	11	1,764	3,264	228	0.02	196	-3.77	-4.19	-4.48
Chlorpyrifos	2921-88-2	350.6	-3.90	5.20	14	1,800	5,376	274	0.07	320	-3.67	-3.93	-5.92

Figure S1: Standard figures for 3 chemicals which exceed the threshold for ϕ3.
a) 3,9-dibromo-7H-benzo[de]anthracen-7-one, b) 1,2,3,4-tetrachlorobenzene, and c) 2,2'-di(propan-2-yl)biphenyl (see S1 for explanation of legends). See explanation of figure below.



Explanation of the standard figures used for visualization. A technique for the visualization of results was introduced by Breivik et al.[2] to offer a more comprehensive mechanistic interpretation of model predictions for individual chemicals (Figures S2 and S3). For each chemical, results are presented for each of the three emission scenarios (100% to air, 100% to water and 100% soil) as identified under the x-axis. Each figure consists of two plots that are stacked on top of each other. The large upper part has the unit of log ϕ along the y-axis. The green, blue and red markers present the predicted emission fractions by emission scenario, i.e. ϕ1, ϕ2, and ϕ3, respectively. The highest value for each LRTP metric across emission scenarios provides the final output. Stipulated lines are included to make a distinction as to whether the predicted metric of interest is above the threshold for POP-like behavior or not (see Table 1 in the main manuscript). The lower part of each figure consists of stacked bars that are scaled from 0% to 100%. Using the emission scenario for air as an example (left part of each figure), the left bar displays the relative significance of LRAT (yellow) and LRWT (light blue) in controlling the predicted dispersion (ϕ1). The middle bar shows the relative importance of net transfer (ϕ2) to water (blue) and soil (red), whereas the right bar highlights the portion accumulating (ϕ3) in soil (red) and water (blue) for each emission scenario.

Figure S2: Standard figures for 6 selected chemicals which exceed the threshold for ϕ3 but not CTD-P_{OV} / TE-P_{OV}.

a) Docosanamide, b) Bromoform, c) 1-chloro-2-[chloro(diphenyl)methyl]benzene, d) 1,1,1,3,3,3-hexafluoropropan-2-ol, e) 1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro-1,4:5,8-dimethanonaphthalene, and f) 1,2,3,4,7,8-hexabromocyclodecane (see S1 for explanation of legends). See explanation of figure below Fig S1.

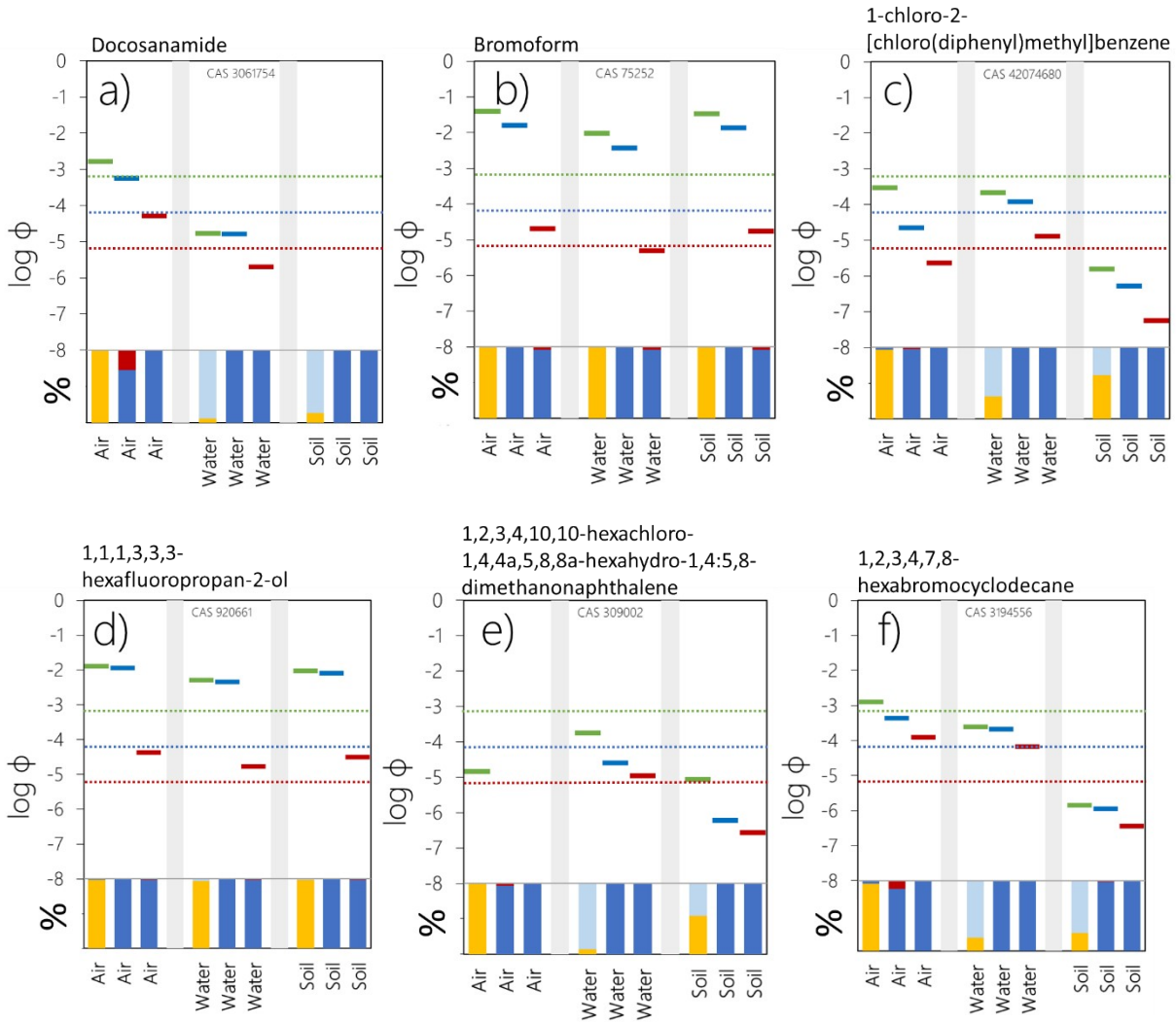


Figure S3: Diagnostic plots for those chemicals which exceed the threshold for TE-P_{OV} but not ϕ3 (N=59).
The plot to the left shows results in a chemical partitioning space plot, whereas the plot to the right shows the results when plotting degradation half-life in air (hours) versus degradation half-life in water (hours). The colors of the markers identify chemicals which accumulate in surface media in the remote region (i) because of LRAT and with a log K_{OA}>11 (grey), and (ii) because of LRAT and with a log K_{OA}<11 (green).

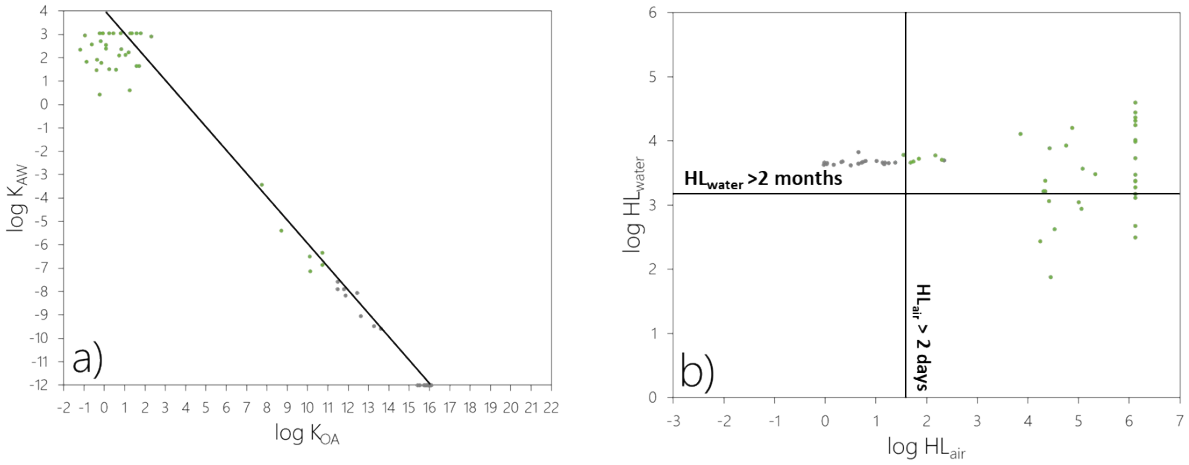


Figure S4: Comparison of the number of chemicals in the screening data set which exceed the criteria for ϕ1, ϕ2, and ϕ3.

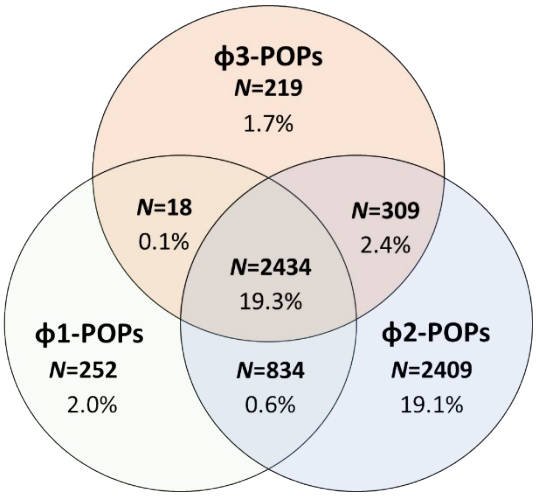
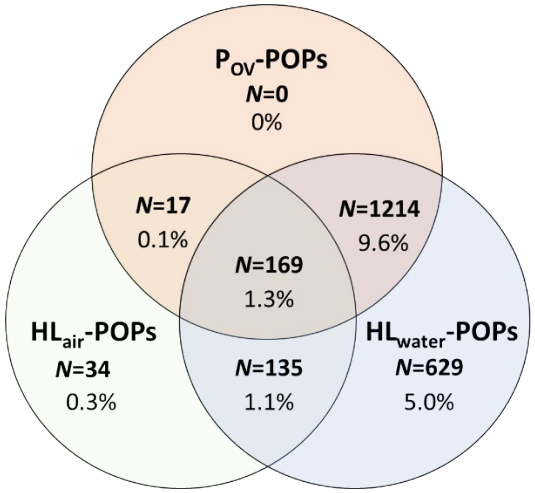


Figure S5: Comparison of the number of chemicals that exceed the threshold for overall persistence and degradation half-lives among the 2,980 chemicals that exceed the criteria for ϕ3 (N=2,198).



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